

National Center for Computational Sciences Snapshot

The Week of December 3, 2007

NOAA Calls on DOE Supercomputers to Simulate Climate and Severe Weather

High-resolution models may improve regional and long-term forecasts

The National Oceanic and Atmospheric Administration (NOAA) aims to understand and predict changes in the global environment. A scientific agency of the Department of Commerce, it charts sea and sky, warns of dangerous weather (through its National Weather Service program), guides the use of coastal and marine resources, and conducts studies to better our stewardship of the environment. Increasingly, improved forecasts depend on complex models run on terascale supercomputers, which carry out trillions of operations each second. Now NOAA is making use of Department of Energy (DOE) leadership computing facilities at Oak Ridge National Laboratory (ORNL) to increase its predictive power with simulations that began in 2007 and will continue into 2008.

“We now have models that are highly scalable and are limited only by available hardware,” says Venkatramani Balaji of NOAA’s Geophysical Fluid Dynamics Laboratory at Princeton University. “DOE’s proposal to make available the Leadership Computing Facility for this project provides an unprecedented match between capability computing resources and a state-of-the-art model.”

The Intergovernmental Panel on Climate Change, corecipient with Al Gore of the 2007 Nobel Peace Prize, employed models that resolve oceanic and atmospheric events on 100-kilometer scales. Using new, higher-resolution models that reveal events at 25-kilometer or finer scales, NOAA researchers may learn if climate variability is predictable on the order of decades and if models can forecast regional phenomena, such as hurricanes. The researchers also expect future models to simulate full cloud physics—missing from current models.

Besides studying the averaged weather conditions that, over time, constitute climate, NOAA scientists are using state-of-the-art models to investigate more immediate severe-weather events. For example, high-resolution simulations of less than a kilometer may reveal how hurricanes are born and evolve. In 2007 NOAA ported existing models to DOE’s high-performance computing (HPC) environment at the National Center for Computational Sciences (NCCS). Its goals for 2008 include optimizing computational performance and evaluating high-resolution forecasts. Knowledge gained from this work may guide national policy for weather-forecasting models in coming years. Simulations may bring real-world benefits.

Says NOAA’s Stephen Lord, “Improved forecasts of severe weather, including hurricane track and intensity on 1- to 7-day time scales and basin-wide hurricane genesis on monthly time scales and other major rainfall and wind events on monthly time scales, result in the savings of life, mitigation of property damage, and an enhanced national economy.”

ORNL Successful at SC07

Laboratory front and center at premier supercomputing conference

Once again ORNL enjoyed tremendous success at SC07 (short for Supercomputing 2007), the premier international symposium for HPC, networking, storage, and analysis.

ORNL's Becky Verastegui was the general chair of the conference, and several ORNL researchers served in key committee positions. ORNL's Gregory Pike was a cowinner of the Bandwidth Challenge for *Using the Data Capacitor for Remote Data Collection, Analysis, and Visualization*.

The laboratory's booth featured all-electronic content displaying the latest breakthroughs in alternative energy solutions, astrophysics, climate modeling, and fusion energy and previewed the future of supercomputing: petascale science.

The booth, which featured several keynote speakers, enjoyed strong attendance and introduced the National Institute for Computational Sciences, a collaboration between the University of Tennessee and ORNL in response to the university's recent \$65 million award from the National Science Foundation.

"The SC conference continues to be the showcase for high-performance computing," said Jack Dongarra, a professor in the Innovative Computing Laboratory at the University of Tennessee. "The conference continues to grow and provide a 'homecoming' for the HPC community. From an excellent technical program to tutorials to workshops to panels along with exhibits, it provides the premier conference for high-performance computing, networking, storage, and analysis."

Two members of ORNL's NCCS User Assistance and Outreach Group, Don Frederick and Bobby Whitten, hosted a "birds-of-a-feather" entitled "HPC Centers and Services." Birds-of-a-feather are semi-informal get-togethers to discuss common issues, said Frederick. Four major supercomputing centers made presentations at the session: the National Energy Research Scientific Computing Center, the Pittsburgh Supercomputing Center, the NCCS, and National Center for Atmospheric Research. According to Frederick, about 35 attendees were present, and the group concluded the meeting by agreeing to continue discussions and collaborations electronically through a mailing list or bulletin board to ensure continued communication on important issues.

Jaguar Upgrades Begin in December

New system to be capable of 275 teraflops

Researchers using ORNL's Jaguar supercomputer will soon get another boost as upgrades to the system make it capable of up to 275 trillion calculations a second (275 teraflops).

The upgrade will replace nearly 8,000 dual-core processors with 2.2-gigahertz AMD quad-core processors, bringing the Cray XT4 system to more than 31,000 processing cores in 84 cabinets. When the project is completed, Jaguar's performance will more than double from the current peak of 119 teraflops.

The project, which will begin in December, is expected to take about 2 months. During this time, Jaguar users will have access to a number of Cray XT4 cabinets that are not part of the upgrade.

Forum to Upgrade MPI Standard

Facelift due by 2010

Rich Graham from the NCCS Technology Integration Group is coordinating an effort to update the decade-old Message Passing Interface (MPI) standard for highly parallel computing.

Graham and others interested in the effort got together at the recent SC07 meeting in Reno, Nevada, and will meet again January 14–16 in Chicago. The group will continue meeting every 8 weeks over the next 2 years to create versions 2.1, 2.2, and 3.0 for the standard, which handles data transfer and dynamic-process control for parallel computers.

The MPI standard is the ubiquitous application programming interface used in parallel simulations. According to Graham, the group expects to complete the three-step upgrade process by 2010, voting in any agreed-upon corrections and changes as the process proceeds.

Graham said the group is strongly encouraging anyone who relies on MPI to get involved. This includes end users, hardware and software vendors, researchers, and MPI implementers.

“MPI has been extremely successful in enabling advances in simulation over the past decade and will continue to play a key role in this arena,” said Graham. “However, with a large body of hands-on experience and a rapidly changing computing ecosystem, it is time to take a look at adjusting the standard to meet this ever-changing environment.”

For more information or to get involved, please visit the MPI Forum website (www.mpi-forum.org), sign up for the mailing list, or get involved in person.

NCCS Holds Blue Gene/P Workshop

New system shows promise for materials, biochemistry

The NCCS recently held a workshop to educate users on the finer points of its newly acquired IBM Blue Gene/P supercomputer.

The new system shows promise in several areas, including biochemistry and materials, and was recently ranked number five on the Green500 list, an inventory of the world's most energy-efficient supercomputers.

The workshop, cosponsored by IBM and held at the American Museum of Science and Energy in Oak Ridge, Tennessee, introduced attendees to the architectural design, programming environment, and possible applications of the Blue Gene/P system.

"The workshop was well attended, and all of the participants were eager to hear what the speaker had to say," said Bobby Whitten, a member of the User Assistance and Outreach Group at the NCCS and the workshop's organizer.